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On the Exact Distributions of the Extreme Roots of the Wishart and MANOVA Matrices

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In this paper, the authors derived exact central distributions of the extreme roots of the Wishart and MANOVA matrices. The expressions for these distributions and the associated probability integrals are written as linear combinations of the products of certain double integrals. The double integrals encountered can be evaluated without any difficulty.

1. INTRODUCTION

The distributions of the extreme roots of the Wishart and multivariate analysis of variance (MANOVA) matrices play an important role in the application of certain test procedures. The joint density of the latent roots of the MANOVA matrix was derived independently by Fisher [2], Hsu [4], and Roy [12]. The cumulative distribution functions (c.d.f.'s) of the extreme roots of the MANOVA matrix were first studied by Roy [13]. He expressed the c.d.f.'s in terms of pseudodeterminants and derived reduction formulas for them; reduction formulas for some pseudodeterminants were also given in [9]. But the exact evaluations of these c.d.f.'s are complicated even by making use of these reduction formulas. Here we note that it is known [8] that the joint density of the latent roots of the Wishart matrix is a limiting form of the density of the roots of MANOVA matrix, and so the expressions for the c.d.f.'s of the extreme roots of the Wishart matrix, in terms of the pseudodeterminants, are implicit in the corresponding expressions

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for the MANOVA matrix. Exact expressions for the p.d.f.'s of the extreme roots of the MANOVA matrix and the largest root of the Wishart matrix are available in the literature [10, 14–16] in terms of zonal polynomials. These expressions are infinite series (except for some special cases) and each term in the series involves zonal polynomials. No analytical bounds are available on the errors of truncations of these series and some empirical evidence indicates that these series converge very slowly. Recently, Krishnaiah and Chang [5] derived an expression involving zonal polynomials for the distribution of the smallest root of the Wishart matrix for a special case; also, an alternative expression[1] involving zonal polynomials is given by Khatri (unpublished)[1] for this case using a different method. Throughout this paper, we restrict our discussion to the exact and central cases only, and so no reference is made to any work on non-central cases.

In the present paper, we give exact expressions for the p.d.f.'s and probability integrals of the distributions of the extreme roots of the Wishart and MANOVA matrices by making use of an elegant method of Mehta [6] for the evaluation of certain integral. The expressions obtained here are linear combinations of the products of certain double integrals which can be evaluated without any difficulty. The merit of the expressions, given in this paper, for the evaluation of the probability integrals, can be illustrated by comparing the expression in Eq. (3.6) with the corresponding (complicated) expressions in [3] and [17], where the expression in [3] is based upon certain reduction formulas of pseudodeterminants and the expression in [17] is based on zonal polynomials.

2. Preliminaries

The inverse and determinant of a square matrix M are denoted by M^{-1} and $|M|$, respectively, whereas the transpose of the matrix N is denoted by N'.

If $A = (a_{ij})$ is a skew-symmetric matrix (that is, $A = -A'$) and A is of even order (say, $2m$), then $|A|^{1/2}$ is known as a Pfaffian. It is also known [7, p. 194] that the Pfaffian can be expressed as a polynomial as follows:

$$m!\,|A|^{1/2} = \sum \pm a_{i_1 i_2} a_{i_3 i_4} \cdots a_{i_{2m-1} i_{2m}}, \tag{2.1}$$

where the summation is over all permutations $i_1, \ldots, i_{2m}$ of $1, 2, \ldots, 2m$ subject to the restrictions $i_1 < i_2$, $i_3 < i_4, \ldots, i_{2m-1} < i_{2m}$, and the sign is positive or negative according as the permutation is even or odd; here we note that the number of distinct terms in the sum on the right side of (2.1) is equal to $1 \cdot 3 \cdots (2m-1)$. We need the following notations in the sequel.

[1] Constantine and Venables (unpublished) also obtained the same expression as Khatri.

Let

$$\rho(\psi; q, r, L, U) = \int_{L\leqslant x_1\leqslant\cdots\leqslant x_q\leqslant U}\cdots\int \prod_{i=1}^{q}\{x_i^r\psi(x_i)\} \prod_{i>j}^{q}(x_i - x_j) \prod_{i=1}^{q} dx_i, \quad (2.2)$$

$$F_s^t = \int_L^U F_s(\theta)\, \theta^t\psi(\theta)\, d\theta, \qquad F_s(\theta) = \int_L^\theta \psi(x)x^s\, dx,$$

and

$$f_s^t = F_s^t - F_t^s. \quad (2.3)$$

In addition, let

$$\Delta(\psi; 2m, r, L, U) = |(a_{ij})_{i,j=1,2,\ldots,2m}|^{1/2}, \quad (2.4)$$

and let $G_t(\psi; 2m+1, r, L, U)$ denote the Pfaffian $|A_t|^{1/2}$, where

$$A_t = (a_{ij})_{i,j=1,2,\ldots,t-1,t+1,\ldots,2m+1}, \qquad \text{and} \qquad a_{ij} = f_{i+r-1}^{j+r-1}.$$

We need the following lemma in the sequel.

Lemma 2.1. *Let $\psi(x)$ be a function of x such that the integral given in* (2.2) *exists, and let $L < U$ and $r \geqslant 0$ be real constants. Then*

$$\rho(\psi; q, r, L, U) = \Delta(\psi; 2m, r, L, U) \qquad \textit{when} \quad q = 2m, \quad (2.5)$$

and

$$\rho(\psi; q, r, L, U) = \sum_{i=0}^{2m}(-1)^i F_{r+i}(U)\, G_{i+1}(\psi; 2m+1, r, L, U)$$

$$\textit{when} \quad q = 2m+1. \quad (2.6)$$

Mehta [6] proved Eq. (2.5) when $\psi(x) = \exp(-x^k)$, and k is a positive integer. Following the same lines as in [6], it is seen that Eq. (2.5) holds true for any $\psi(x)$ as long as the integral exists. We will sketch the method briefly below. When $q = 2m$, we integrate out $x_1, x_3, \ldots, x_{2m-1}$ on the right side of (2.2) and, after simplification, obtain the following:

$$\rho(\psi; 2m, r, L, U) = \int_R\cdots\int \prod_{i=1}^{m}\psi(x_{2i})\, \eta(x_2, x_4, \ldots, x_{2m}) \prod_{i=1}^{m} dx_{2i} \quad (2.7)$$

where the region of integration is $R : L \leqslant x_2 \leqslant x_4 \leqslant \cdots \leqslant x_{2m} \leqslant U$, and

$$\eta(x_2, x_4, \dots, x_{2m}) = \begin{vmatrix} F_r(x_2) & x_2^r & F_r(x_4) & x_4^r & \cdots & F_r(x_{2m}) & x_{2m}^r \\ F_{r+1}(x_2) & x_2^{r+1} & F_{r+1}(x_4) & x_4^{r+1} & \cdots & F_{r+1}(x_{2m}) & x_{2m}^{r+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ F_{r+2m-1}(x_2) & x_2^{r+2m-1} & F_{r+2m-1}(x_4) & x_4^{r+2m-1} & \cdots & F_{r+2m-1}(x_{2m}) & x_{2m}^{r+2m-1} \end{vmatrix}.$$

Since the integrand in (2.7) is a symmetric function of $x_2, x_4, \dots, x_{2m}$, we can write (2.7) as

$$\rho(\psi; 2m, r, L, U) = \frac{1}{m!} \int \cdots \int_{R^*} \prod_{i=1}^{m} \psi(x_{2i})\, \eta(x_2, x_4, \dots, x_{2m}) \prod_{i=1}^{m} dx_{2i}, \quad (2.8)$$

where the region of integration is $R^* : L \leqslant x_{2i} \leqslant U$, $i = 1, 2, \dots, m$. Now, following the same lines as in Appendix A.7 of [7], we obtain the desired result. When $q = 2m + 1$ and $\psi(x) = \exp(-x^k)$, Mehta [6] made an ambiguous statement that "the case of odd q requires only slight additional care, the final results are however unchanged." So, we will briefly sketch below the proof of Eq. (2.6). As in [6], we write

$$\rho(\psi; 2m+1, r, L, U) = \int \cdots \int_{R} \prod_{i=1}^{m} \psi(x_{2i})$$

$$\times \begin{vmatrix} F_r(x_2) & x_2^r & F_r(x_4) & x_4^r & \cdots & F_r(U) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ F_{r+2m}(x_2) & x_2^{r+2m} & F_{r+2m}(x_4) & x_4^{r+2m} & \cdots & F_{r+2m}(U) \end{vmatrix} \prod_{i=1}^{m} dx_{2i}. \quad (2.9)$$

Now, let D_i denote the determinant obtained by deleting the last column and $(i + 1)$-th row in the determinant on the right side of (2.9). Then

$$\rho(\psi; 2m+1, r, L, U) = \sum_{i=0}^{2m} (-1)^i F_{r+i}(U) \int \cdots \int_{R} D_i \prod_{j=1}^{m} \{\psi(x_{2j})\, dx_{2j}\}. \quad (2.10)$$

Here we note that each D_i is of even order, and the integrand in each of the multiple integrals in the right side of (2.10) is a symmetric function of $x_2, x_4, \dots, x_{2m}$. Now using the same argument as in the case of q even, we observe that Eq. (2.6) is true.

Equations (2.5) and (2.6) can be simplified by using Eq. (2.1).

3. Distributions of the Extreme Roots of the Wishart Matrix

Let X be a $p \times n$ matrix whose columns are distributed independently as multivariate normal with zero mean vector and covariance matrix Σ. Also, let $S = XX'$. In this section, we assume that $\Sigma = I_p$ where I_p is the identity matrix. Also, let $l_1 < l_2 < \cdots < l_p$ be the latent roots of S. Then, it is well known that the joint density of $l_1, \ldots, l_p$ is given by

$$f_1(l_1, \ldots, l_p) = k(p, n) \prod_{i=1}^{p} [l_i^r \exp(-l_i/2)] \prod_{i>j}^{p} (l_i - l_j), \tag{3.1}$$

where $r = (n - p - 1)/2$ and

$$k(p, n) = \pi^{p/2}(1/2)^{np/2} \Big/ \prod_{i=1}^{p} [\Gamma((n + 1 - i)/2)\, \Gamma((p + 1 - i)/2)].$$

In (3.1), making the transformations $g_i = l_i/l_1$, $(i = 2, \ldots, p)$, $l_1 = l_1$ and integrating out $g_2, \ldots, g_p$, we get

$$f_2(l_1) = k(p, n) \exp(-l_1/2) l_1^{rp+(p-1)(1+(p/2))} \tag{3.2}$$

$$\times \int \cdots \int_{1 \leqslant g_2 \leqslant \cdots \leqslant g_p < \infty} \exp\left[-l_1 \sum_{i=2}^{p} g_i/2\right] \prod_{i=2}^{p} [g_i^r(g_i - 1)] \prod_{i>j=2}^{p} (g_i - g_j) \prod_{i=2}^{p} dg_i .$$

The above integral can be evaluated by using Lemma 2.1. So, we have the following result:

Theorem 3.1. *The distribution of the smallest root l_1 of the Wishart matrix S is given by*

$$f_2(l_1) = k(p, n) l_1^{rp+(p-1)(1+(p/2))} \exp(-l_1/2)\, \rho(\psi_1 ; p - 1, r, 1, \infty),$$
$$0 < l_1 < \infty \tag{3.3}$$

where $\rho(\psi_1; p - 1, r, 1, \infty)$ is given by (2.5) *or* (2.6) *according as* $(p - 1)$ *is even or odd, and* $\psi_1(x) = \exp(-l_1 x/2)(x - 1)$.

To compute the c.d.f. of l_1, we note that

$$F_2(c, p, n) = P[l_1 \leqslant c] = 1 - P[\infty \geqslant l_p \geqslant l_{p-1} \geqslant \cdots \geqslant l_1 \geqslant c].$$

So, applying Lemma 2.1, we obtain the following:

Remark 3.1. The c.d.f of the smallest root of the Wishart matrix S is given by

$$F_2(c, p, n) = 1 - k(p, n)\,\rho(\psi_2; p, r, c, \infty), \tag{3.4}$$

where $\rho(\psi_2; p, r, c, \infty)$ is given by (2.5) or (2.6) according as p is even or odd, and $\psi_2(x) = \exp(-x/2)$.

We will now discuss about the distribution of the largest root of the Wishart matrix. In (3.1), making the transformations $h_i = l_i/l_p$, $l_p = l_p$, $(i = 1, 2,..., p - 1)$ and applying Lemma 2.1 to integrate out $h_1,..., h_{p-1}$, we obtain the following:

THEOREM 3.2. *The distribution of the largest root l_p of the Wishart matrix S is given by*

$$f_3(l_p) = k(p, n) l_p^{rp+(p-1)(1+(p/2))} \exp(-l_p/2)\,\rho(\psi_3\,; p - 1, r, 0, 1), \qquad 0 < l_p < \infty \tag{3.5}$$

where $\rho(\psi_3; p - 1, r, 0, 1)$ is given by (2.5) or (2.6) according as $(p - 1)$ is even or odd, and $\psi_3(x) = \exp(-l_p x/2)(1 - x)$.

By using Lemma 2.1, we obtain easily Eq. (3.6) given below.

Remark 3.2. The probability integral of the joint density of l_1 and l_p is given by

$$P[L \leqslant l_1 \leqslant l_p \leqslant U] = k(p, n)\,\rho(\psi_2; p, r, L, U), \tag{3.6}$$

where $\rho(\psi_2; p, r, L, U)$ is given by Eq. (2.5) or (2.6), according as p is even or odd. In particular, if $L = 0$, Eq. (3.6) gives the c.d.f. of l_p.

The Pfaffians which appear in Eqs. (3.3)–(3.6) can be simplified by using Eq. (2.1). So, basically, the computations of the expressions in Eqs. (3.3)–(3.6) involve evaluation of certain double integrals which can be evaluated without any difficulty. Since the expressions obtained in this section are in terms of the functions of the form $\rho(\psi; q, r, L, U)$, we will write $\rho(\psi; q, r, L, U)$ explicitly for $q = 2, 3, 4$ below for illustration:

$$\rho(\psi; 2, r, L, U) = f_r^{r+1},$$

$$\rho(\psi; 3, r, L, U) = F_r(U) f_{r+1}^{r+2} - F_{r+1}(U) f_r^{r+2} + F_{r+2}(U) f_r^{r+1},$$

$$\rho(\psi; 4, r, L, U) = f_r^{r+1} f_{r+2}^{r+3} - f_r^{r+2} f_{r+1}^{r+3} + f_r^{r+3} f_{r+1}^{r+2},$$

where

$$f_s^t = \int_L^U \psi(\theta)\{F_s(\theta)\theta^t - F_t(\theta)\theta^s\}\, d\theta, \qquad F_s(c) = \int_L^c \psi(x)x^s\, dx.$$

Wigner and other nuclear physicists are very much interested (e.g., [1, 7, 11, 18])[2] in the distribution problems connected with the eigenvalues of certain random matrices. In particular, they are interested in the random matrix A and its complex analog where the elements of A are independently and normally distributed with zero means and the variances of the diagonal elements are equal to 2, whereas the variances of the off-diagonal elements are equal to 1. They call the distribution of A as Wishart distribution, whereas, in the statistical literature, the distribution of S is known as Wishart distribution. But the techniques used by them are useful in solving certain distribution problems that arise in multivariate statistical analysis.

4. Distributions of the Extreme Roots of the MANOVA Matrix

Let S_1 and S_2 be independently distributed as $p \times p\,(p \leqslant n_1, n_2)$ central Wishart matrices with n_1 and n_2 degrees of freedom, and let $E(S_1/n_1) = E(S_2/n_2) = \Sigma$. Also, let $\theta_p > \theta_{p-1} > \cdots > \theta_1$ be the latent roots of $S_1(S_1 + S_2)^{-1}$. Then, it is well known [2, 4, 12] that the joint density of $\theta_1, ..., \theta_p$ is

$$f_4(\theta_1, ..., \theta_p) = C(p, r, n) \prod_{i=1}^{p} \{\theta_i^r(1-\theta_i)^n\} \prod_{i>j}^{p} (\theta_i - \theta_j),$$

$$1 > \theta_p > \theta_{p-1} > \cdots > \theta_1 > 0, \tag{4.1}$$

where

$$C(p, r, n) = \frac{\pi^{p^2/2}\Gamma_p(r+n+p+1)}{\{\Gamma_p((2r+p+1)/2)\,\Gamma_p((2n+p+1)/2)\,\Gamma_p(p/2)\}},$$

$$\Gamma_p(a) = \pi^{p(p-1)/4} \prod_{i=1}^{p} \Gamma(a - \tfrac{1}{2}(i-1)),$$

$$r = (n_1 - p - 1)/2 \qquad \text{and} \qquad n = (n_2 - p - 1)/2.$$

If we make the transformations $h_i^* = \theta_i/\theta_p$, $(i = 1, 2, ..., p-1)$ and $\theta_p = \theta_p$ in (4.1) and integrate out $h_1^*, ..., h_{p-1}^*$ applying Lemma 2.1, we obtain the following result:

[2] The authors wish to thank Professor E. P. Wigner for bringing these references to their attention.

THEOREM 4.1. *The distribution of the largest root* θ_p *of the* MANOVA *matrix* $S_1(S_1 + S_2)^{-1}$ *is given by*

$$f_5(\theta_p) = C(p, r, n)\theta_p^{rp+(p-1)(1+(p/2))}(1 - \theta_p)^n \rho(\psi_4 ; p - 1, r, 0, 1),$$
$$0 < \theta_p < 1 \quad (4.2)$$

where $\psi_4(x) = (1 - x\theta_p)^n(1 - x)$.

The distribution of θ_1 can be obtained [8] from that of θ_p by changing θ_p to $1 - \theta_1$, and interchanging r and n.

Using Lemma 2.1, we obtain the following results also:

Remark 4.1. The probability integral of the joint density of θ_1 and θ_p is given by

$$P[L \leqslant \theta_1 \leqslant \theta_p \leqslant U] = C(p, r, n)\, \rho(\psi_5; p, r, L, U), \quad (4.3)$$

where $\psi_5(x) = (1 - x)^n$. When $L = 0$, the right side of (4.3) is the c.d.f. of θ_p.

Remark 4.2. Let $F_5(c, p, r, n)$ be the c.d.f. of the smallest root θ_1. Then

$$F_5(c, p, r, n) = P[\theta_1 \leqslant c] = 1 - C(p, r, n)\, \rho(\psi_5; p, r, c, 1). \quad (4.4)$$

The Pfaffians which appear in (4.2)–(4.4) can be simplified further by using Eq. (2.1). So, the computations of the expressions in (4.2)–(4.4) involve the computation of certain double integrals which can be evaluated without difficulty.

If $n_2 \geqslant p \geqslant n_1$, then it is known that the joint density of the roots of $S_1(S_1 + S_2)^{-1}$ is obtained from (4.1) by interchanging p and n_1, and changing n_2 to $n_1 + n_2 - p$. So, when $n_2 \geqslant p \geqslant n_1$, the distributions of the extreme roots of the MANOVA matrix are easily obtained from the corresponding expressions when $p \leqslant n_1, n_2$.

5. GENERAL REMARKS

In general, let the joint density of the roots of a random matrix be of the form

$$f(\lambda_1, \ldots, \lambda_p) = C \prod_{i=1}^{p} \psi(\lambda_i) \prod_{i<j} (\lambda_i - \lambda_j), \qquad a \leqslant \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_p \leqslant b, \quad (5.1)$$

where a, b and C are known constants.

Then, we have the following:

$$P[a \leqslant \lambda_1 \leqslant \lambda_p \leqslant b] = C\rho(\psi; p, 0, a, b)$$

$$P[\lambda_1 \leqslant c] = 1 - C\rho(\psi; p, 0, c, b),$$

$$P[\lambda_p \leqslant c] = C\rho(\psi; p, 0, a, c),$$

where $\rho(\psi; p, 0, L, U)$ can be evaluated using Lemma 2.1. The p.d.f.'s of λ_1 and λ_p can be obtained, of course, by differentiating the c.d.f.'s or by suitable transformations of variables in (5.1).

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